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Redetermination of the crystal structure of the crystal sponge the poly[tetrakis(μ_3 -2,4,6-tris(pyridin-4-yl)-1,3,5-triazine)-dodecaiodido-hexazinc(II) nitrobenzene solvate], $C_{72}H_{48}I_{12}N_{24}Zn_6 \cdot 10(C_6H_5NO_2)$

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Abstract

$C_{132}H_{98}I_{12}N_{34}O_{20}Zn_6$, monoclinic, $P2_1c$, $a = 34.97800(15)$ Å, $b = 15.02541(6)$ Å, $c = 30.13247(12)$ Å, $\beta = 101.9033(4)^\circ$, $V = 15,495.86(11)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0501$, $wR_{\text{ref}}(F^2) = 0.1329$, $T = 95$ K.

CCDC no.: 2118557.

Asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The crystals were prepared according to the published procedure for preparation of poly(bis(μ_3 -2,4,6-tris(4-pyridyl)-1,3,5-triazine)-hexakisiodo-trizinc nitrobenzene solvate) [5]. The resulting material is a mixture of expected crystals [5] and title compound.

Experimental details

The H atoms were refined with soft restraints ($C-H$ 0.93–0.98 Å) and $U_{\text{iso}}(H)$ (1.2–1.5 $U_{\text{eq}}(C)$), and then refined with riding constraints. The disordered iodide anions attached to Zn16 were refined using thermal similarity and occupancy sum restraints, resulting in final occupancy ratio of 820(7):180(7). The structure is a redetermination of crystal structure deposited with the CCDC [6]. The structure was a part of a thesis work not a peer reviewed journal. Therefore, the information on sample preparation and model refinement is lacking. Furthermore the disorder of iodide anions was missing in the structure and nitrobenzene molecules were severely distorted.

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Table 1: Data collection and handling.

Crystal:	Prism, colourless
Size:	$0.21 \times 0.15 \times 0.08$ mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ :	20.39 mm ⁻¹
Diffractometer, scan mode:	SuperNova, φ and ω -scans
$\theta_{\max}$, completeness:	74.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	268,201, 31,402, 0.043
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 30257
$N(\text{param})_{\text{refined}}$:	1857
Programs:	CrysAlis ^{PRO} [1], SUPERFLIP [2], CRYSTALS [3], DIAMOND [4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.91298 (2)	0.14033 (5)	0.26527 (3)	0.0187
I2	0.973586 (12)	0.04184 (3)	0.288425 (14)	0.0242
I3	0.867226 (13)	0.12167 (3)	0.188376 (14)	0.0266
Zn4	0.61592 (3)	0.32508 (6)	0.46251 (3)	0.0246
I5	0.627886 (14)	0.47197 (3)	0.424449 (17)	0.0337
I6	0.600615 (14)	0.30765 (4)	0.540701 (15)	0.0342
Zn7	0.33546 (3)	0.35761 (6)	0.09556 (3)	0.0253
I8	0.367867 (17)	0.47845 (3)	0.057323 (18)	0.0410
I9	0.275953 (14)	0.38338 (3)	0.130870 (15)	0.0322
Zn10	0.13381 (2)	-0.34865 (6)	-0.06260 (3)	0.0200
I11	0.151423 (13)	-0.49301 (3)	-0.098684 (16)	0.0284
I12	0.118202 (13)	-0.33546 (3)	0.015898 (14)	0.0263
Zn13	-0.16209 (2)	-0.38479 (5)	-0.42105 (3)	0.0182
I14	-0.130337 (13)	-0.49828 (3)	-0.464480 (14)	0.0265
I15	-0.213739 (13)	-0.40804 (3)	-0.373365 (14)	0.0269
Zn16	0.44177 (3)	-0.09036 (7)	-0.22754 (4)	0.0356
I17 ^a	0.41454 (7)	-0.05478 (17)	-0.30916 (5)	0.0494
I18 ^a	0.50263 (6)	-0.01339 (11)	-0.17795 (9)	0.0458
I19 ^b	0.3998 (4)	-0.0833 (4)	-0.31403 (17)	0.0466
I20 ^b	0.4943 (3)	-0.0153 (5)	-0.1955 (4)	0.0495
N1	0.81681 (15)	-0.0221 (4)	0.43007 (18)	0.0187
C2	0.80715 (18)	0.0520 (4)	0.4056 (2)	0.0173
N3	0.77796 (15)	0.1070 (4)	0.40936 (18)	0.0199
C4	0.75995 (18)	0.0863 (4)	0.4430 (2)	0.0186
N5	0.76838 (15)	0.0168 (4)	0.47145 (18)	0.0190
C6	0.79574 (17)	-0.0370 (4)	0.4613 (2)	0.0162
C7	0.83145 (19)	0.0745 (4)	0.3723 (2)	0.0198
C8	0.86822 (18)	0.0381 (4)	0.3769 (2)	0.0191
C9	0.89128 (19)	0.0613 (4)	0.3469 (2)	0.0194
N10	0.87908 (16)	0.1177 (4)	0.31234 (17)	0.0197
C11	0.8430 (2)	0.1523 (4)	0.3072 (2)	0.0223
C12	0.8183 (2)	0.1333 (4)	0.3366 (2)	0.0221
C13	0.72701 (18)	0.1447 (4)	0.4490 (2)	0.0208
C14	0.7063 (2)	0.1926 (6)	0.4129 (2)	0.0324
C15	0.6750 (2)	0.2426 (6)	0.4190 (3)	0.0363
N16	0.66355 (17)	0.2478 (4)	0.45855 (19)	0.0255
C17	0.68401 (19)	0.2020 (5)	0.4937 (2)	0.0224
C18	0.71564 (19)	0.1491 (4)	0.4904 (2)	0.0229

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C19	0.80298 (18)	-0.1221 (4)	0.4869 (2)	0.0169
C20	0.83105 (19)	-0.1808 (4)	0.4778 (2)	0.0201
C21	0.83804 (19)	-0.2596 (4)	0.5027 (2)	0.0206
N22	0.81867 (15)	-0.2792 (4)	0.53568 (17)	0.0194
C23	0.79103 (19)	-0.2232 (4)	0.5437 (2)	0.0218
C24	0.78239 (18)	-0.1439 (4)	0.5200 (2)	0.0183
N31	0.47994 (17)	0.0446 (4)	0.32453 (19)	0.0240
C32	0.4820 (2)	0.1335 (5)	0.3218 (2)	0.0257
N33	0.46189 (18)	0.1849 (4)	0.2892 (2)	0.0303
C34	0.4374 (2)	0.1409 (5)	0.2572 (2)	0.0260
N35	0.43248 (17)	0.0524 (4)	0.25536 (19)	0.0253
C36	0.4553 (2)	0.0079 (5)	0.2895 (2)	0.0252
C37	0.5114 (2)	0.1791 (5)	0.3575 (2)	0.0257
C38	0.5317 (2)	0.1337 (5)	0.3952 (2)	0.0267
C39	0.5611 (2)	0.1779 (5)	0.4246 (2)	0.0272
N40	0.57116 (17)	0.2630 (4)	0.41790 (19)	0.0256
C41	0.5509 (2)	0.3057 (5)	0.3815 (3)	0.0308
C42	0.5206 (2)	0.2675 (5)	0.3513 (3)	0.0328
C43	0.4145 (2)	0.1918 (5)	0.2184 (2)	0.0276
C44	0.4037 (3)	0.2776 (6)	0.2241 (3)	0.0499
C45	0.3816 (3)	0.3212 (6)	0.1876 (3)	0.0459
N46	0.37206 (18)	0.2867 (4)	0.1454 (2)	0.0294
C47	0.3814 (2)	0.2019 (5)	0.1417 (3)	0.0342
C48	0.4024 (2)	0.1513 (5)	0.1769 (3)	0.0334
C49	0.4532 (2)	-0.0899 (5)	0.2866 (2)	0.0260
C50	0.4320 (2)	-0.1306 (5)	0.2480 (3)	0.0357
C51	0.4305 (3)	-0.2215 (6)	0.2451 (3)	0.0406
N52	0.4495 (2)	-0.2746 (4)	0.2782 (2)	0.0323
C53	0.4707 (2)	-0.2352 (5)	0.3151 (3)	0.0364
C54	0.4735 (3)	-0.1457 (5)	0.3208 (3)	0.0369
N61	0.27940 (16)	-0.0237 (4)	-0.03647 (19)	0.0215
C62	0.30616 (19)	0.0360 (4)	-0.0422 (2)	0.0198
N63	0.32769 (16)	0.0343 (4)	-0.07355 (17)	0.0194
C64	0.32147 (19)	-0.0376 (4)	-0.1007 (2)	0.0199
N65	0.29434 (15)	-0.1002 (4)	-0.09967 (18)	0.0203
C66	0.27429 (18)	-0.0890 (4)	-0.0670 (2)	0.0206
C67	0.31135 (19)	0.1140 (4)	-0.0112 (2)	0.0199
C68	0.28425 (19)	0.1342 (4)	0.0148 (2)	0.0229
C69	0.2906 (2)	0.2071 (5)	0.0435 (2)	0.0232
N70	0.32279 (18)	0.2575 (4)	0.04785 (18)	0.0231
C71	0.3491 (2)	0.2382 (5)	0.0224 (2)	0.0296
C72	0.3446 (2)	0.1676 (5)	-0.0076 (2)	0.0260
C73	0.34706 (19)	-0.0483 (4)	-0.1337 (2)	0.0202
C74	0.3712 (2)	0.0212 (5)	-0.1412 (2)	0.0250
C75	0.3971 (2)	0.0058 (5)	-0.1692 (2)	0.0275
N76	0.39949 (17)	-0.0725 (4)	-0.18991 (19)	0.0250
C77	0.3746 (2)	-0.1377 (5)	-0.1839 (2)	0.0254
C78	0.3484 (2)	-0.1289 (4)	-0.1564 (2)	0.0235
C79	0.24220 (18)	-0.1527 (4)	-0.0654 (2)	0.0196
C80	0.2306 (2)	-0.2145 (5)	-0.1000 (2)	0.0258
C81	0.1991 (2)	-0.2686 (4)	-0.0980 (2)	0.0242
N82	0.18009 (16)	-0.2662 (4)	-0.06376 (19)	0.0220
C83	0.1921 (2)	-0.2071 (5)	-0.0302 (2)	0.0257
C84	0.2224 (2)	-0.1497 (5)	-0.0300 (2)	0.0261
N91	-0.01728 (15)	-0.0862 (3)	-0.18907 (17)	0.0176
C92	-0.00901 (17)	-0.1724 (4)	-0.19574 (19)	0.0149

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
N93	-0.02679 (15)	-0.2223 (3)	-0.23036 (17)	0.0175
C94	-0.05460 (18)	-0.1822 (4)	-0.2596 (2)	0.0171
N95	-0.06598 (15)	-0.0968 (4)	-0.25678 (18)	0.0191
C96	-0.04565 (17)	-0.0523 (4)	-0.2212 (2)	0.0159
C97	0.02370 (18)	-0.2148 (4)	-0.16310 (19)	0.0164
C98	0.0467 (2)	-0.1661 (4)	-0.1287 (2)	0.0229
C99	0.0779 (2)	-0.2086 (4)	-0.1004 (2)	0.0229
N100	0.08682 (15)	-0.2936 (3)	-0.10606 (17)	0.0182
C101	0.0643 (2)	-0.3405 (4)	-0.1396 (2)	0.0247
C102	0.03235 (19)	-0.3037 (4)	-0.1684 (2)	0.0232
C103	-0.07523 (18)	-0.2326 (4)	-0.3001 (2)	0.0163
C104	-0.07391 (18)	-0.3249 (4)	-0.3026 (2)	0.0195
C105	-0.09645 (19)	-0.3677 (4)	-0.3395 (2)	0.0193
N106	-0.11880 (16)	-0.3219 (3)	-0.37427 (17)	0.0181
C107	-0.1175 (2)	-0.2329 (4)	-0.3728 (2)	0.0237
C108	-0.09659 (19)	-0.1858 (4)	-0.3371 (2)	0.0204
C109	-0.05497 (19)	0.0444 (4)	-0.2204 (2)	0.0196
C110	-0.08863 (19)	0.0760 (4)	-0.2490 (2)	0.0235
C111	-0.0961 (2)	0.1663 (4)	-0.2502 (2)	0.0236
N112	-0.07208 (15)	0.2262 (3)	-0.22618 (18)	0.0194
C113	-0.03946 (19)	0.1952 (4)	-0.1982 (2)	0.0213
C114	-0.03016 (19)	0.1051 (5)	-0.1943 (2)	0.0221
C201	0.9811 (2)	-0.3426 (5)	0.5336 (3)	0.0302
C202	1.0185 (2)	-0.3715 (6)	0.5513 (3)	0.0349
C203	1.0403 (2)	-0.4044 (6)	0.5222 (3)	0.0424
C204	1.0251 (3)	-0.4071 (6)	0.4756 (3)	0.0419
C205	0.9871 (3)	-0.3768 (6)	0.4587 (3)	0.0372
C206	0.9647 (2)	-0.3441 (5)	0.4877 (3)	0.0329
N207	0.95749 (19)	-0.3061 (4)	0.5644 (2)	0.0324
O208	0.97070 (16)	-0.3098 (4)	0.60555 (17)	0.0364
O209	0.92586 (15)	-0.2720 (4)	0.54765 (18)	0.0339
C211	0.9731 (2)	-0.1075 (5)	0.4824 (2)	0.0270
C212	0.9421 (2)	-0.0712 (5)	0.4982 (3)	0.0366
C213	0.9467 (3)	-0.0576 (6)	0.5446 (3)	0.0511
C214	0.9811 (4)	-0.0806 (6)	0.5734 (3)	0.0548
C215	1.0115 (3)	-0.1172 (6)	0.5571 (3)	0.0487
C216	1.0082 (2)	-0.1301 (5)	0.5112 (3)	0.0354
N217	0.96967 (19)	-0.1200 (4)	0.4337 (2)	0.0300
O218	0.99626 (19)	-0.1567 (5)	0.4207 (2)	0.0492
O219	0.93966 (17)	-0.0934 (4)	0.40822 (19)	0.0401
C221	0.8724 (2)	-0.1916 (5)	0.3352 (2)	0.0251
C222	0.8896 (2)	-0.1578 (5)	0.3013 (2)	0.0268
C223	0.8673 (2)	-0.1018 (5)	0.2694 (2)	0.0302
C224	0.8290 (2)	-0.0828 (5)	0.2713 (2)	0.0309
C225	0.8128 (2)	-0.1168 (5)	0.3054 (3)	0.0309
C226	0.8343 (2)	-0.1725 (5)	0.3384 (3)	0.0310
N227	0.89567 (19)	-0.2513 (4)	0.3690 (2)	0.0298
O228	0.92387 (18)	-0.2892 (4)	0.3597 (2)	0.0411
O229	0.88564 (18)	-0.2601 (4)	0.40567 (19)	0.0405
C231	0.5974 (3)	-0.1173 (8)	0.6068 (4)	0.0579
C232	0.5772 (6)	-0.1012 (13)	0.5646 (6)	0.1113
C233	0.5712 (8)	-0.006 (2)	0.5556 (7)	0.1630
C234	0.5840 (6)	0.0555 (11)	0.5898 (9)	0.1113
C235	0.6049 (5)	0.0308 (11)	0.6340 (7)	0.0957
C236	0.6093 (3)	-0.0570 (9)	0.6402 (5)	0.0659

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
N237	0.6052 (3)	-0.2166 (9)	0.6181 (5)	0.0848
O238	0.6037 (4)	-0.2607 (9)	0.5829 (7)	0.1623
O239	0.6149 (4)	-0.2334 (12)	0.6575 (6)	0.1503
C241	0.5215 (4)	0.6896 (9)	0.4909 (5)	0.0757
C242	0.5420 (5)	0.6211 (9)	0.4728 (4)	0.0782
C243	0.5523 (4)	0.5488 (10)	0.5013 (5)	0.0818
C244	0.5434 (4)	0.5426 (9)	0.5427 (4)	0.0672
C245	0.5257 (4)	0.6090 (10)	0.5599 (5)	0.0794
C246	0.5149 (3)	0.6844 (9)	0.5345 (5)	0.0677
N247	0.5108 (5)	0.7647 (9)	0.4599 (8)	0.1356
O248	0.5160 (8)	0.7653 (12)	0.4214 (4)	0.2356
O249	0.4984 (4)	0.8302 (9)	0.4802 (6)	0.1367
C251	0.7099 (2)	-0.0120 (6)	0.2412 (3)	0.0390
C252	0.6905 (2)	0.0391 (6)	0.2677 (3)	0.0350
C253	0.7000 (3)	0.1276 (7)	0.2724 (3)	0.0520
C254	0.7265 (3)	0.1668 (9)	0.2532 (4)	0.0652
C255	0.7459 (3)	0.1178 (10)	0.2268 (4)	0.0689
C256	0.7387 (3)	0.0274 (10)	0.2202 (3)	0.0592
N257	0.7011 (3)	-0.1060 (6)	0.2357 (3)	0.0545
O258	0.6706 (3)	-0.1325 (5)	0.2437 (2)	0.0635
O259	0.7254 (3)	-0.1546 (7)	0.2225 (4)	0.1007
C261	0.8254 (3)	0.4816 (6)	0.4036 (3)	0.0369
C262	0.8253 (3)	0.3902 (7)	0.4008 (3)	0.0556
C263	0.8562 (4)	0.3501 (7)	0.3843 (3)	0.0587
C264	0.8830 (3)	0.4042 (8)	0.3689 (3)	0.0523
C265	0.8819 (3)	0.4944 (8)	0.3728 (4)	0.0603
C266	0.8528 (3)	0.5331 (7)	0.3899 (4)	0.0560
N267	0.7942 (3)	0.5273 (7)	0.4216 (3)	0.0523
O268	0.7700 (2)	0.4795 (7)	0.4342 (3)	0.0776
O269	0.7937 (3)	0.6086 (6)	0.4216 (3)	0.0740
C271	0.7070 (3)	0.5067 (6)	0.1251 (3)	0.0432
C272	0.6913 (3)	0.5286 (7)	0.0810 (3)	0.0508
C273	0.6885 (3)	0.6171 (7)	0.0693 (3)	0.0533
C274	0.7005 (3)	0.6815 (7)	0.1013 (4)	0.0540
C275	0.7153 (3)	0.6610 (7)	0.1460 (3)	0.0506
C276	0.7190 (3)	0.5720 (6)	0.1581 (3)	0.0436
N277	0.7104 (3)	0.4130 (6)	0.1380 (3)	0.0550
O278	0.7002 (3)	0.3567 (6)	0.1086 (3)	0.0881
O279	0.7233 (3)	0.3937 (6)	0.1785 (3)	0.0814
C281	0.7968 (2)	0.4865 (6)	0.2519 (3)	0.0422
C282	0.8133 (3)	0.5123 (6)	0.2178 (4)	0.0464
C283	0.8178 (3)	0.6023 (8)	0.2108 (4)	0.0551
C284	0.8059 (3)	0.6640 (7)	0.2392 (4)	0.0579
C285	0.7888 (3)	0.6374 (8)	0.2735 (4)	0.0643
C286	0.7841 (3)	0.5474 (7)	0.2813 (3)	0.0523
N287	0.7917 (2)	0.3907 (6)	0.2600 (3)	0.0531
O288	0.8070 (2)	0.3386 (6)	0.2389 (3)	0.0732
O289	0.7726 (3)	0.3686 (6)	0.2879 (3)	0.0709
C291	0.6809 (3)	0.4711 (7)	0.2924 (4)	0.0569
C292	0.6746 (3)	0.5264 (8)	0.2567 (4)	0.0605
C293	0.6819 (4)	0.6142 (9)	0.2635 (5)	0.0687
C294	0.6960 (4)	0.6482 (8)	0.3047 (6)	0.0729
C295	0.7036 (4)	0.5921 (13)	0.3413 (4)	0.0860
C296	0.6960 (4)	0.4993 (10)	0.3351 (4)	0.0756
N297	0.6726 (4)	0.3727 (8)	0.2841 (4)	0.0806

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
O298	0.6603 (3)	0.3469 (8)	0.2479 (4)	0.1029
O299	0.6803 (5)	0.3265 (7)	0.3189 (5)	0.1357
H91	0.9168	0.0368	0.3508	0.0267*
H81	0.8774	-0.0031	0.4006	0.0234*
H181	0.7293	0.1169	0.5159	0.0296*
H171	0.6765	0.2062	0.5222	0.0280*
H411	0.5582	0.3651	0.3763	0.0391*
H421	0.5062	0.3003	0.3264	0.0415*
H381	0.5251	0.0740	0.4009	0.0335*
H391	0.5754	0.1468	0.4502	0.0361*
H481	0.4083	0.0905	0.1728	0.0404*
H471	0.3733	0.1740	0.1131	0.0422*
H691	0.2716	0.2218	0.0608	0.0297*
H681	0.2616	0.0986	0.0131	0.0277*
H721	0.3635	0.1552	-0.0253	0.0323*
H711	0.3718	0.2743	0.0252	0.0384*
H781	0.3314	-0.1765	-0.1526	0.0297*
H771	0.3754	-0.1923	-0.1995	0.0320*
H531	0.4846	-0.2724	0.3385	0.0429*
H541	0.4893	-0.1212	0.3474	0.0465*
H501	0.4190	-0.0954	0.2232	0.0432*
H511	0.4150	-0.2481	0.2189	0.0484*
H751	0.4140	0.0526	-0.1742	0.0331*
H741	0.3699	0.0775	-0.1272	0.0301*
H801	0.2437	-0.2192	-0.1245	0.0342*
H811	0.1906	-0.3098	-0.1219	0.0300*
H991	0.0931	-0.1763	-0.0759	0.0264*
H981	0.0415	-0.1049	-0.1247	0.0294*
H1021	0.0164	-0.3386	-0.1913	0.0304*
H1011	0.0707	-0.4009	-0.1439	0.0301*
H1141	-0.0072	0.0852	-0.1742	0.0272*
H1131	-0.0224	0.2368	-0.1804	0.0272*
H1111	-0.1197	0.1871	-0.2688	0.0300*
H1101	-0.1060	0.0362	-0.2677	0.0299*
H1081	-0.0964	-0.1226	-0.3374	0.0245*
H1071	-0.1321	-0.2006	-0.3978	0.0311*
H211	0.8572	-0.3000	0.4965	0.0272*
H201	0.8451	-0.1674	0.4548	0.0255*
H241	0.7627	-0.1054	0.5264	0.0230*
H231	0.7770	-0.2378	0.5666	0.0263*
H1051	-0.0966	-0.4309	-0.3403	0.0252*
H1041	-0.0574	-0.3577	-0.2793	0.0262*
H831	0.1789	-0.2050	-0.0056	0.0332*
H841	0.2299	-0.1080	-0.0061	0.0321*
H451	0.3722	0.3790	0.1924	0.0555*
H441	0.4112	0.3063	0.2526	0.0545*
H151	0.6606	0.2745	0.3938	0.0468*
H141	0.7138	0.1914	0.3843	0.0405*
H121	0.7931	0.1595	0.3322	0.0269*
H111	0.8341	0.1912	0.2824	0.0297*
H2121	0.9185	-0.0553	0.4778	0.0465*
H2131	0.9259	-0.0325	0.5563	0.0630*
H2141	0.9840	-0.0708	0.6051	0.0668*
H2151	1.0348	-0.1341	0.5776	0.0624*
H2161	1.0294	-0.1537	0.4997	0.0423*
H2021	1.0289	-0.3681	0.5830	0.0436*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H2031	1.0659	-0.4266	0.5340	0.0547*
H2041	1.0405	-0.4288	0.4554	0.0536*
H2051	0.9766	-0.3784	0.4270	0.0461*
H2061	0.9388	-0.3237	0.4768	0.0424*
H2221	0.9156	-0.1735	0.2996	0.0335*
H2231	0.8786	-0.0754	0.2465	0.0383*
H2241	0.8138	-0.0457	0.2489	0.0373*
H2251	0.7865	-0.1029	0.3063	0.0393*
H2261	0.8233	-0.1958	0.3622	0.0376*
H2661	0.8513	0.5961	0.3921	0.0669*
H2621	0.8049	0.3557	0.4087	0.0673*
H2631	0.8590	0.2872	0.3844	0.0713*
H2521	0.6715	0.0140	0.2824	0.0435*
H2531	0.6868	0.1629	0.2906	0.0657*
H2541	0.7313	0.2288	0.2573	0.0787*
H2551	0.7651	0.1462	0.2134	0.0884*
H2561	0.7526	-0.0064	0.2020	0.0749*
H2761	0.7300	0.5555	0.1885	0.0535*
H2751	0.7223	0.7062	0.1682	0.0611*
H2741	0.6992	0.7420	0.0920	0.0700*
H2731	0.6774	0.6330	0.0388	0.0627*
H2721	0.6828	0.4836	0.0590	0.0603*
H2861	0.7725	0.5273	0.3055	0.0614*
H2821	0.8213	0.4694	0.1984	0.0561*
H2831	0.8294	0.6214	0.1866	0.0677*
H2921	0.6652	0.5037	0.2270	0.0747*
H2931	0.6774	0.6529	0.2380	0.0803*
H2461	0.5037	0.7340	0.5466	0.0827*
H2641	0.9024	0.3772	0.3554	0.0627*
H2841	0.8102	0.7255	0.2348	0.0704*
H2361	0.6212	-0.0797	0.6692	0.0772*
H2941	0.7000	0.7105	0.3083	0.0807*
H2851	0.7797	0.6808	0.2917	0.0763*
H2651	0.9013	0.5299	0.3634	0.0713*
H2961	0.7014	0.4588	0.3598	0.0860*
H2431	0.5648	0.5001	0.4902	0.0887*
H2421	0.5491	0.6277	0.4442	0.0938*
H2441	0.5500	0.4898	0.5600	0.0780*
H2351	0.6155	0.0736	0.6564	0.1046*
H2451	0.5207	0.6047	0.5896	0.0933*
H2951	0.7141	0.6155	0.3706	0.1030*
H2341	0.5771	0.1156	0.5823	0.1336*
H2321	0.5693	-0.1455	0.5421	0.1407*
H2331	0.5576	0.0111	0.5262	0.1727*

The overall R factor was > 9%; therefore, the structure model presented here is a significant improvement related to the deposited structure.

Comment

Since their discovery [7], the crystal sponges have received a lot of attention worldwide for their ability to provide structural

information on hard to crystallize or non-crystalline compounds. The method has seen success in the field of natural compounds [8, 9], and pharmaceutical substances [10]. The crystal structure of title compound is presented in the Figure. The asymmetric unit consists of six ZnI_2 nodes connecting four TPT ligands forming the crystal framework and 10 nitrobenzene molecules. The non-hydrogen atoms forming the asymmetric unit are depicted with APDs drawn at 50% probability level. The single bonds within TPT ligands allow rotation of the pyridine rings, resulting in dihedral angles between mean planes through 1,3,5-triazine and pyridine rings ranging from $4.4(3)$ to $28.0(3)^\circ$. The tilting is closely tied to formation of non-covalent interactions. The Zn(II) cations were found to be in distorted tetrahedral coordination. The distortions are caused by the presence of two iodide anions within the coordination sphere. The Zn–I bond distances do not significantly deviate from the average value $2.55 \text{ \AA}$, only in case of disordered iodides differences up to $0.056 \text{ \AA}$ were observed. The Zn–N bonds were found to be within $0.016 \text{ \AA}$ from the average value of $2.06 \text{ \AA}$. The most significant angular distortions from ideal geometry were observed in I–Zn–I and N–Zn–N angles with average values of 125.06 and 101.93° respectively. Larger variance from the average values was observed with differences of up to 4.23 and 4.20° for I–Zn–I and N–Zn–N respectively. In absence of good hydrogen bond donors and abundance of good hydrogen bond acceptors the non-covalent interactions are dominated by weaker C–H $\cdots$ O and C–H $\cdots$ I hydrogen bonds. All nitrobenzene molecules are acceptors of at least one C–H $\cdots$ O hydrogen bond, while six out of 10 molecules also serve as hydrogen bond donors.

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